Material Property Database and Environmental Attribute Models for NM Science Research

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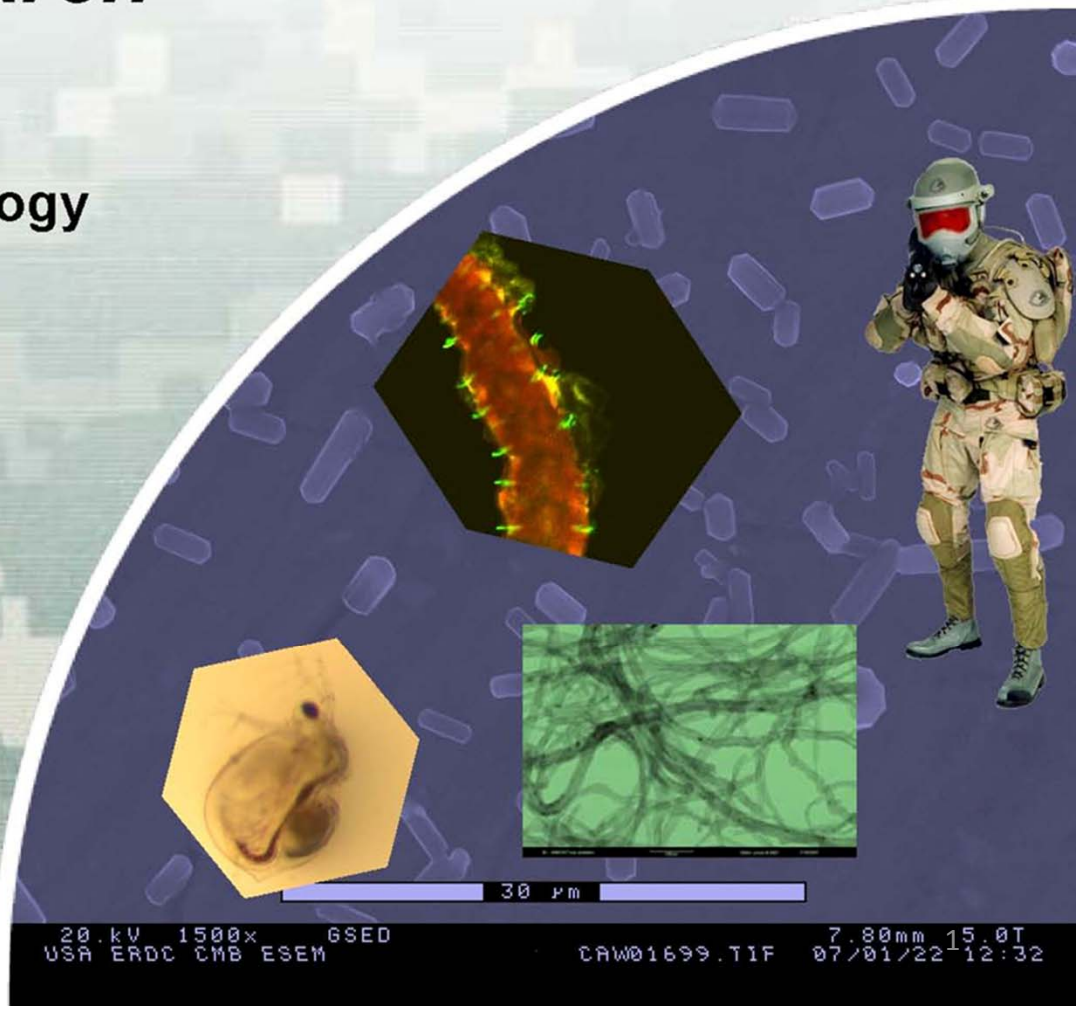

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Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE	2. REPORT TYPE	3. DATES COVERED
28 MAR 2011		**00-00-2011 to 00-00-2011**

4. TITLE AND SUBTITLE	5a. CONTRACT NUMBER
Material Property Database and Environmental Attribute Models for NM Science Research	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **U.S. Army Engineer Research and Development Center,Environmental Laboratory,3909 Halls Ferry Road,Vicksburg,MS,39180-6199**	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

13. SUPPLEMENTARY NOTES
Presented at the 2011 DoD Environmental Monitoring & Data Quality Workshop (EMDQ 2011), 28 Mar ? 1 Apr, Arlington, VA.

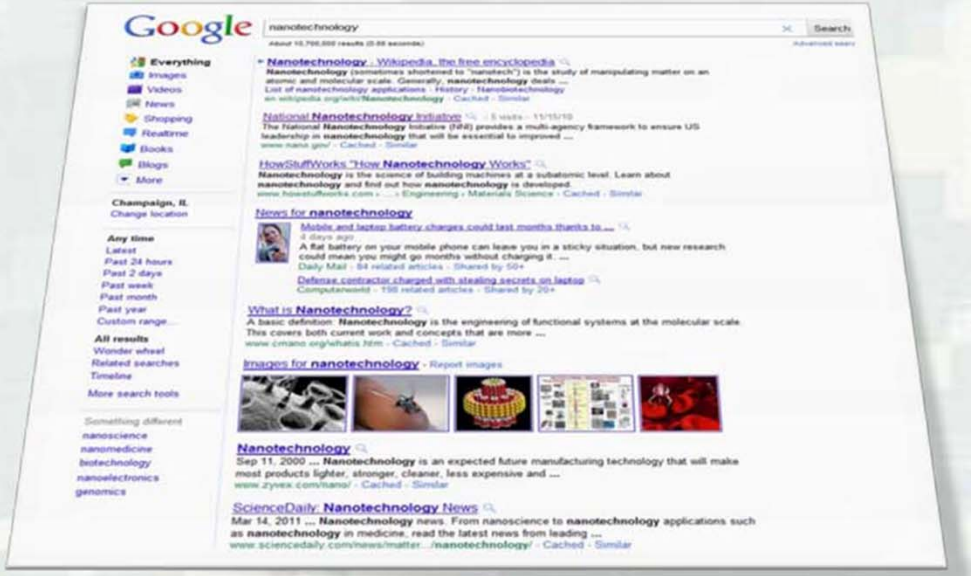
14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**	**Same as Report (SAR)**	**15**	

Challenges in Understanding "Nano"

- Internet
  - 10,700,000 hits on nanotechnology
  - 199,000 hits on nanotoxicology
- Scientists and regulatory agencies have not yet determined what is most important
  - Assessing hazard
  - Regulating
  - Critical parameters



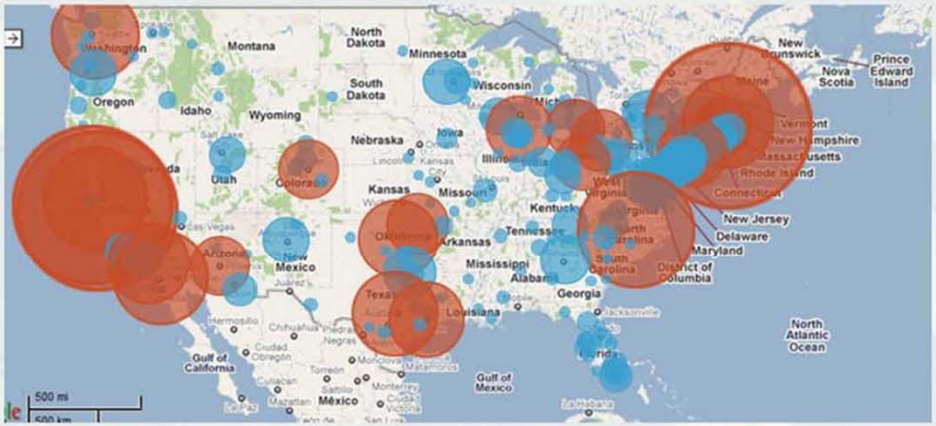
Goals

1. Provide place “to go” for initial information
2. Basic understanding of what types of information you might need to collect or understand
3. How to interpret information gathered from resources
4. What to expect from R&D community and Regulatory community

Consumer and Product Databases

Woodrow Wilson Center, Consumer product database
http://www.nanotechproject.org/inventories/consumer/

Contains references to research papers, articles, and books on (or related to) potential health and environmental risks of nanomaterials sorted by material or compound, body organ or biological effect studied, or other miscellaneous issues.
http://www.nanoceo.net/nanorisks

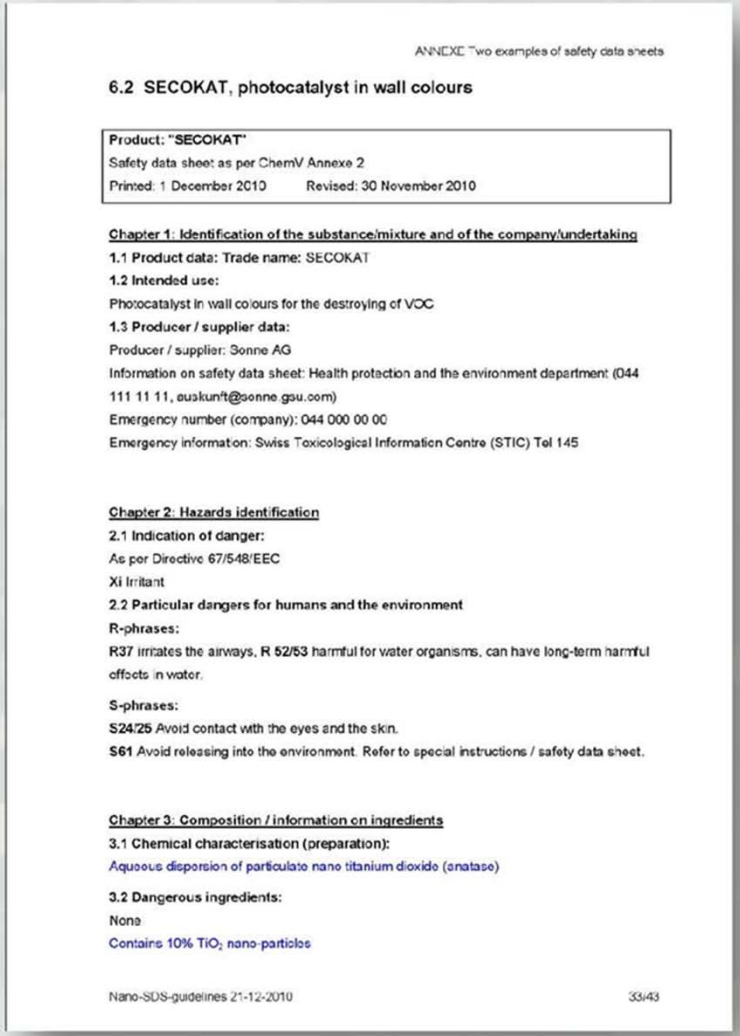


U.S. Nano Metro Map - companies, universities, government laboratories, and organizations working in nanotechnology around the United States

Materials Property and Safety

SAFENANO

UK resource on nanotechnology hazard and risk. Includes a format for nanomaterial specific safety data sheet.
www.safenano.org



ANNEX Two examples of safety data sheets

6.2 SECOKAT, photocatalyst in wall colours

Product: "SECOKAT"
Safety data sheet: as per ChemV Annexe 2
Printed: 1 December 2010 Revised: 30 November 2010

Chapter 1: Identification of the substance/mixture and of the company/undertaking
1.1 Product data: Trade name: SECOKAT
1.2 Intended use:
Photocatalyst in wall colours for the destroying of VOC
1.3 Producer / supplier data:
Producer / supplier: Sonne AG
Information on safety data sheet: Health protection and the environment department: (044 111 11 11, auskunft@sonne.gsu.com)
Emergency number (company): 044 000 00 00
Emergency information: Swiss Toxicological Information Centre (STIC) Tel 145

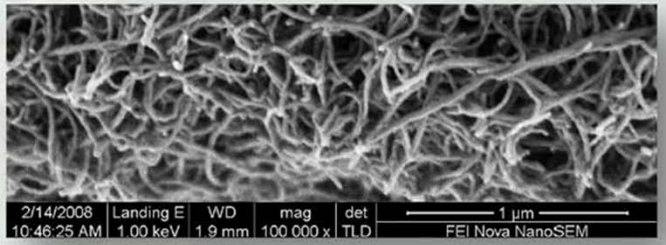
Chapter 2: Hazards identification
2.1 Indication of danger:
As per Directive 67/548/EEC
Xi Irritant
2.2 Particular dangers for humans and the environment
R-phrases:
R37 irritates the airways, **R 52/53** harmful for water organisms, can have long-term harmful effects in water.
S-phrases:
S24/25 Avoid contact with the eyes and the skin.
S61 Avoid releasing into the environment. Refer to special instructions / safety data sheet.

Chapter 3: Composition / information on ingredients
3.1 Chemical characterisation (preparation):
Aqueous dispersion of particulate nano titanium dioxide (anatase)
3.2 Dangerous ingredients:
None
Contains 10% TiO_2 nano-particles

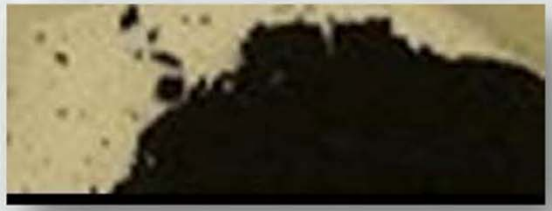
Nano-SDS-guidelines 21-12-2010 33/43

What Properties are Important?

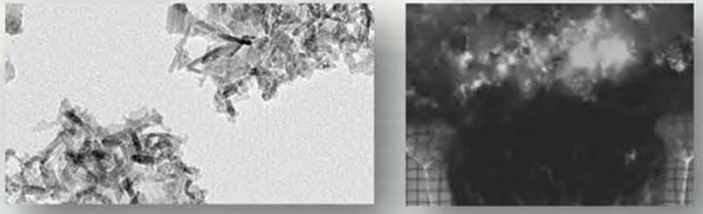
- Carbon
  - MWCNT, SWCNT, Fullerene, Waste
- Aluminum
  - Explosive, propellant
- Silver
  - Coatings, textiles, polymers
- Titanium dioxide
  - Coatings



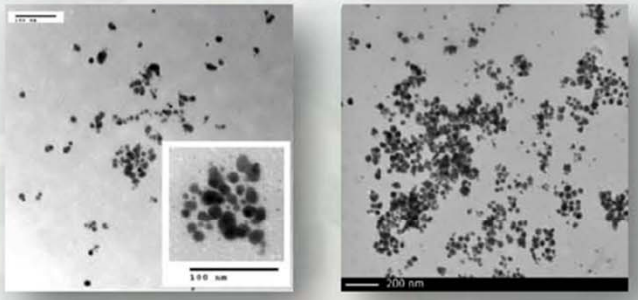
Multi-walled carbon nanotubes



Fullerene soot waste



Nano Al, combined with RDX explosive, sintered form of aluminum oxide after reaction, Carney, Indian Head NRL

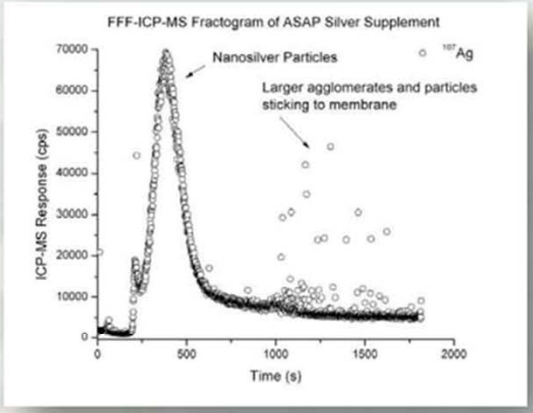


Nano Ag, 10 nm particles and polyvinylpyrrolidone (PVP) capped

* Identified as strategic materials for Army technologies, Shashi Karna, ARL Senior Scientist

Characterization of Materials

- Size
  - Electron microscopy (SEM, TEM)
  - Dynamic light scattering
  - Field Flow Fractionation ICP-MS
- Surface area
  - BET (Brunauer, Emmett and Teller)
- Morphology
  - Electron microscopy
  - Confocal microscopy
  - Nanoindentor (mechanical properties)
- Surface Chemistry
  - Zeta potential
  - Solid-state NMR
  - FTIR / Raman spectroscopy
  - Multispectral fluorometer
  - Auto titrator – zeta potential curves



Field Flow Fractionation, Coupling to ICP-MS/AES allows elemental quantitation as a function of size

Minimum Characterization Standards

- **What does the material look like?**
  - Particle size/size distribution
  - Agglomeration state/Aggregation
  - Shape
- **What is the material made of?**
  - Overall composition (including chemical composition and crystal structure)
  - Surface Composition
  - Purity (including levels of impurities)
- **What factors affect how a material interacts with its surroundings?**
  - Surface Area
  - Surface Chemistry, including reactivity, hydrophobicity
  - Surface Charge

Minimum Characterization Standards

- **Overarching considerations to take into account when characetrizing engineered nanomaterials in toxicity studies:**
  - *Stability—how do material properties change with time (dynamic stability), storage, handling, preparation, delivery etc? Include solubility, and the rate of material release through dissolution.*
  - *Context/Media—how do material properties change in different media; i.e. from the bulk material to dispersions to material in various biological matrices? ("as administered" characterization is considered to be particularly important)*
  - *Where possible, materials should be characterized sufficiently to interpret the response to the amount of material against a range of potentially relevant dose metrics, including mass, surface-area and number concentration.*

Laboratory Safety

National Institute for Occupational Safety and Health
NIOSH

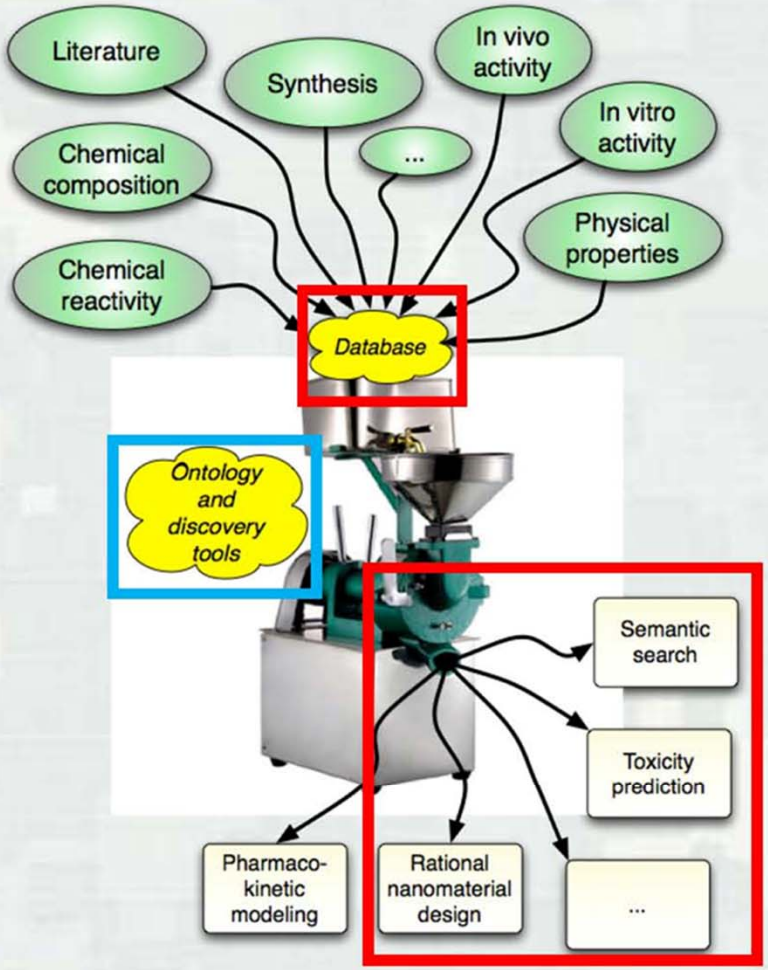
http://www.cdc.gov/niosh/topics/nanotech/default.html

NANOPARTICLE INFORMATION LIBRARY

NIOSH Nanoparticle Information Database. Online database includes: Nanomaterial composition Method of production, Particle size, surface area, and morphology, Demonstrated or intended applications of the nanomaterial, Availability for research or commercial applications, Associated or relevant publications. http://nanoparticlelibrary.net/index.asp

http://www.cdc.gov/niosh/docs/2008-112/pdfs/2008-112.pdf

How do we integrate this information?

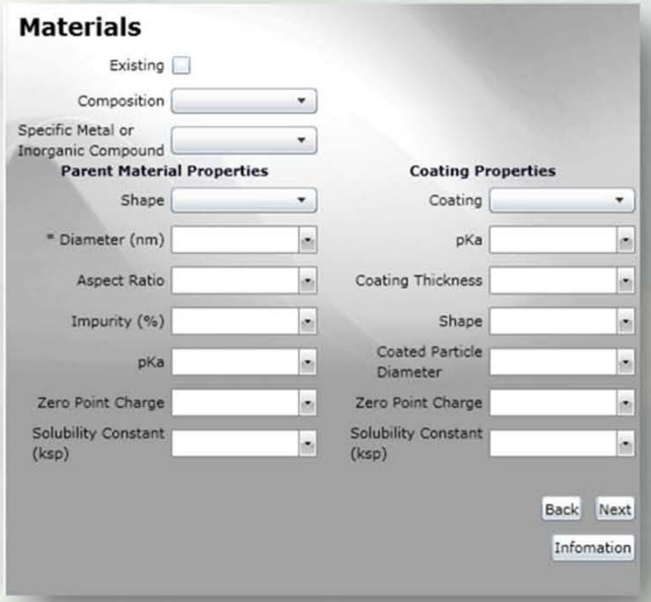


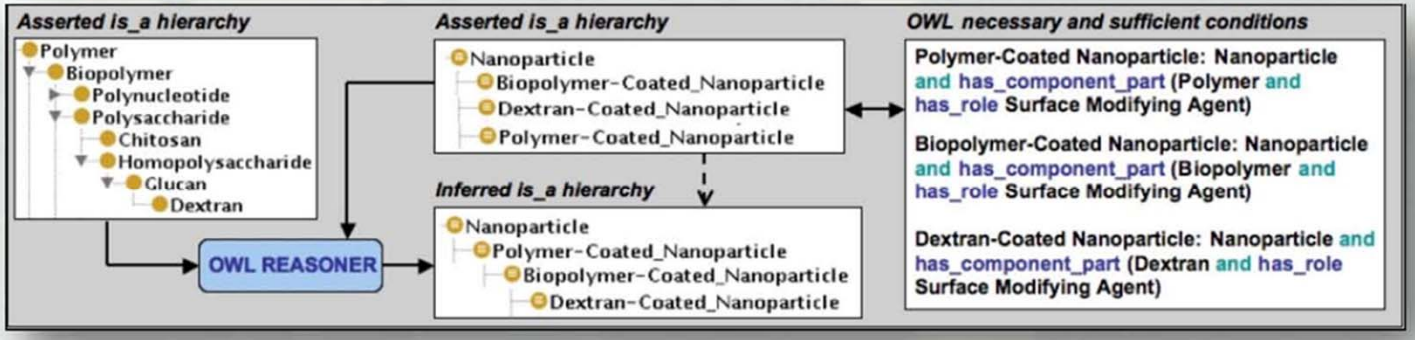
From Nathan Baker, PNL, 2010

- Information from databases (parameters and endpoints) can be integrated via an ontology
- Specification of logical relationships between concepts
- Also usually includes definitions, synonyms, properties, etc.
- Ontology
  - Standard terminology
  - Logical relationships between concepts
  - Classifiers for computer-aided materials design and modeling

Materials Property Database

- Categories, descriptors, properties based on a common ontology
- Develop inferred relationships
- Used to predict attributes through QSAR, QSPR, mechanistic models
- Applications include materials development





Thomas DG, Pappu RV, Baker NA. NanoParticle Ontology for Cancer Nanotechnology Research. *J Biomed Inform,*

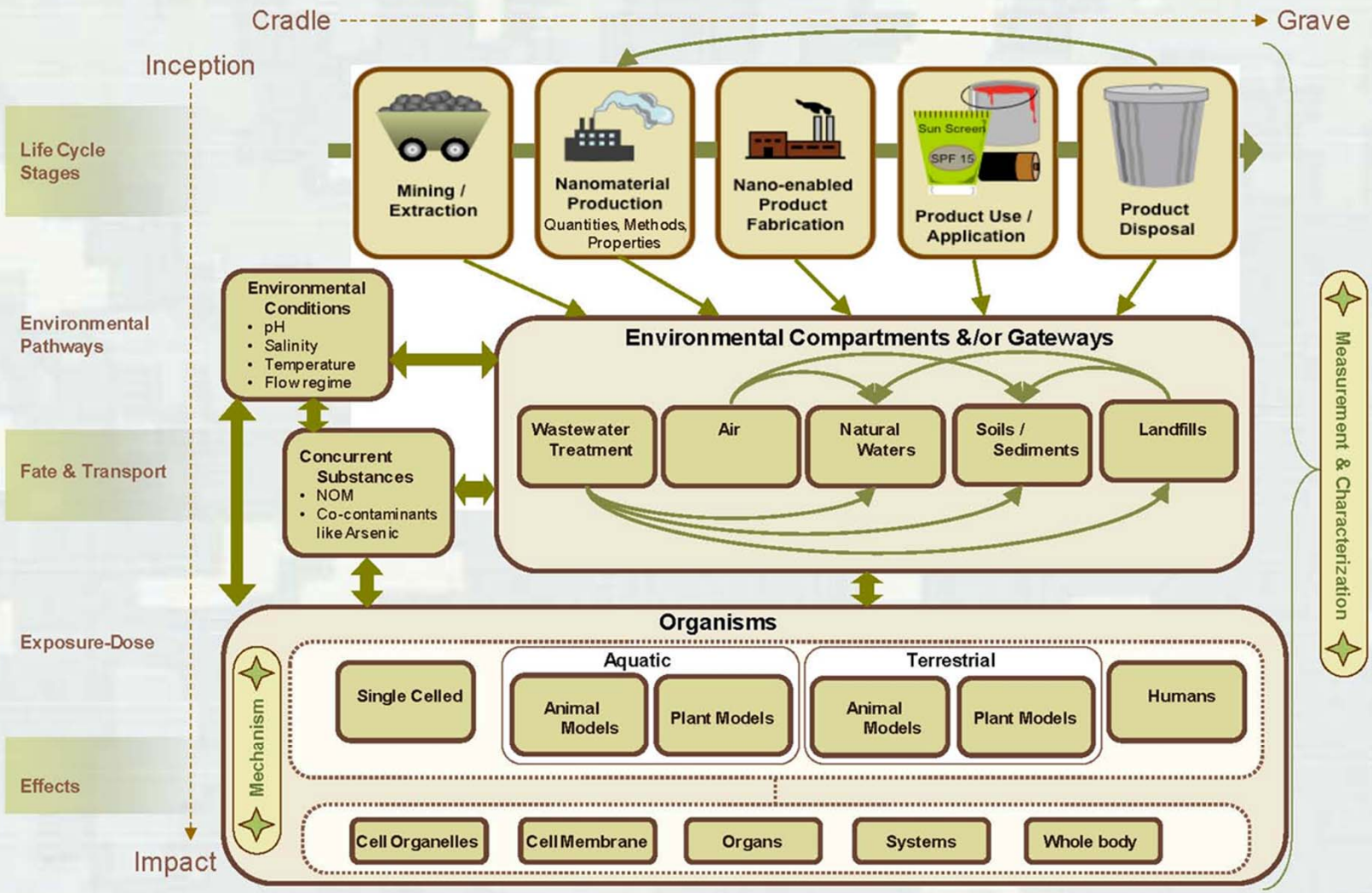
Pacific Northwest NATIONAL LABORATORY

NATIONAL CANCER INSTITUTE

ONAMI

NATIONAL INSTITUTES OF HEALTH

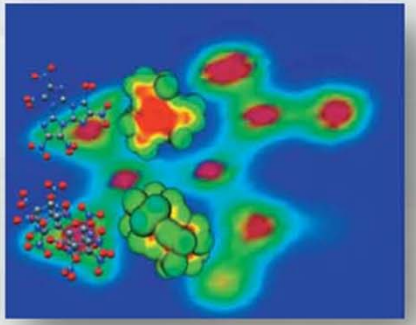
Life Cycle



CEA Process, From Davis 2010

Nanomaterials Hazard Model

- Tool for estimating potential hazards of materials being developed.
- Rely on empirical data when available and modeling approaches for missing/unknown data.
- Components:
  - Materials database
  - Fate calculations
  - Toxicity estimates
  - Hazard diamonds
  - Documentation
- Modeling properties
  - QSPR/QSAR
  - Molecular models



Atomic scale models for prediction based on structure and surface chemistry

Risk Assessment of Engineered Nanomaterials

http://el.erdc.usace.army.mil/nano

Environmental Laboratory, Engineer Research and Development Center, U.S. Army Corps of Engineers

http://el.erdc.usace.army.mil/nano/